Application of a "Spraylet" Model to the Simulation of Fuel Spray Autoignition

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Abstract

Modeling of spray selfignition requires significant simplifications due to the high complexity of the physical and chemical processes involved. A turbulent vaporizing two-phase flow describes the physics of mixture formation through a spray in hot air. When modeling mixing of fuel vapor with the surrounding gas, the difference between diffusion rates of components as well as the finite penetration of the diffusion fluxes must be taken into account. The surrounding of an individual droplet or a group of droplets is characterized through significant inhomogeneity. Such inhomogeneity has a great influence on the characteristics of ignition and combustion. Therewith, a fuel oxidation mechanism defines the scores of components that are involved in a diffusive process. In spite of a significant reduction of chemical kinetics, its calculation requires a high performance of computers. Thus, sub-models of the spray simulation must describe the turbulent large scale flow as well as the detailed small scale diffusive transport including chemical reactions.

In this work a new approach for spray ignition simulation is presented. The simulation is split into two tasks. The initial formation of the spray, atomization, vaporization and turbulent two-phase flow are computed in large scale. Chemistry is not taken into account in this part. From this CFD-calculation the droplet´s trajectories and the gas parameters as temperature and mixture fraction along these trajectories are extracted. The latter serve as variable boundary conditions for the second task, the single droplet ignition simulation, named "Spraylet". The "Spraylet" model is solving the transient differential equations of the processes in the liquid and gas phases with variable physical properties. Also the concept of multi-component diffusion is applied. The effects of the presence of neighboring droplets in the flow, usually referred to as "spray" effects, is approximated by taking modifications of the conditions at the outer boundary of the computational domain into account. Thus the model considers the finite rates of diffusion and chemical reactions, as well as spray effects, and allows for spray ignition simulations to predict the most probable instants of ignition of the individually calculated droplet trajectories. The individual ignition delay times can finally be projected onto its trajectories delivering a spatial plane of the most probable instant of ignition – this independent of whether ignition happens soon (heterogeneous ignition) or later (homogeneous ignition). While the CFD part is handling spray formation, turbulence, temperature, pressure and global vaporization, the "Spraylet" calculations take care of droplet related physics and chemistry.

The "Spraylet" model is an enhancement of former single droplet ignition simulations that were validated through hundreds of microgravity droplet ignition experiments. The validation of the "Spraylet"-based simulation was performed by comparison with experimental data obtained from spray ignition experiments performed in a hot blowdown wind-tunnel. N-heptane as liquid fuel was injected into cross flow of air with a pressure of 5 bar and a temperature of 800 K.

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